An Interoperable, Data-Structure-Neutral Component for Mesh Query and Manipulation

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Much of the effort required to create a new simulation code goes into developing infrastructure for mesh data manipulation, adaptive refinement, design optimization, and so forth. This infrastructure is an obvious target for code re-use, except that implementations of these functionalities are typically tied to specific data structures. In this paper, we describe a software component — an abstract data model and programming interface — designed to provide low-level mesh query and manipulation support for meshing and solution algorithms. The component's data model provides a data abstraction, completely hiding all details of how mesh data is stored, while its interface defines how applications can interact with that data. Because the component has been carefully designed to be general-purpose and efficient, it provides a practical platform for implementing high-level mesh operations independently of the underlying mesh data structures. After describing the data model and interface, we provide several usage examples, each of which has been used successfully with multiple implementations of the interface functionality. The overhead due to accessing mesh data through the interface rather than directly accessing the underlying mesh data is shown to be acceptably small.

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1. INTRODUCTION

Developing new simulation software for problems described by partial differential equations has become a relatively common but nonetheless still laborious task. Much of the effort required to create a new simulation code goes into developing infrastructure for mesh and geometry data manipulation, equation discretization, adaptive refinement, design optimization, and so forth. Because this infrastructure is common to many simulations, re-usable software for these tasks could be shared across many simulation codes and could significantly reduce both the time, effort, and expertise required to develop and maintain new simulation codes.

Currently, *libraries* are the most common mechanism for software re-use in scientific computing, including highly-successful examples for numerical linear algebra [Balay et al. 1997; Balay et al. 2004; EISPACK 2004; LAPACK 2004; LINPACK 2004] and parallel partitioning and load balancing [Devine et al. 2002; Boman et al. 2007; ParMETIS 2008; Walshaw and Cross 2007; Jostle 2002]. A key drawback in using libraries as a mechanism for software re-use is the difficulty in modifying an application already using one library so that it can use another. At a minimum, all symbol names from one library must be changed to names from the other. However, the difficulties really only begin there. Libraries of similar purpose often package functionality in very different ways. Consequently, data structures shared between application and library and even the control flow between application and library may need to be totally re-designed. This need to re-design an application — or portions of it — so that it can re-use some other piece of software is often termed an *impedance mismatch*. The greater the impedance mismatch, the more effort is required to resolve it. This time-consuming re-design process can be a significant diversion from the central scientific investigation, so many application researchers are reluctant to undertake it. As a result, improvements in algorithms often take years to migrate from the research community into application simulations.

Components represent a higher level of abstraction than libraries. To quote from the Common Component Architecture Forum (CCA) website [CCA Forum homepage 2004],

> A **component** is a software object, meant to interact with other components, encapsulating certain functionality or a set of functionalities. A component has a clearly defined interface and conforms to a prescribed behavior common to all components within an architecture....
> The **component interface** is a set of methods supported by a component, and type definitions for the data used for arguments to those methods. An interface itself is a type and can be an argument for a component method.

Essentially, a component defines both a *specification* for an application programming interface (API) and an abstract *data model* defining the semantics of the data that is passed through the interface. Returning to the familiar example of linear algebra, a numerical linear algebra component would define a standard interface for operations such as dot products, matrix-vector multiplication, and linear system solution. Its abstract data model would include objects such as vectors and matrices. A key advantage to components is that any application using a component can, *without modification*, use another implementation of that same component, because all compliant implementations necessarily have equivalent functionality. In other words, software re-use can be achieved with no additional effort.

This paper describes a meshing component intended to support low-level mesh access and manipulation. In addition, this component is designed to support the requirements of solver applications, including the ability to define mesh subsets and to attach arbitrary user data to mesh entities. Finally, our mesh component interface is intended to be both language and data structure independent. In summary, the mesh component we present is intended to support low-level interaction between applications programs — both meshing and solution applications — and external mesh databases regardless of the data structures and programming language used by each.

The most prominent example of prior research in defining interfaces for meshing is the Unstructured Grid Consortium (UGC), a working group of the American Institute for Aeronautics and Astronautics's Meshing, Visualization, and Computing Environments Technical Committee [UGC Consortium 2005]. The first release of the UGC interface [UGC Consortium 2002] was aimed at high level mesh operations, including mesh generation and quality assessment. Recognizing a need for additional and lower-level functionality, the UGC has developed an interface for defining generic high-level services, as well as a low-level query and modification interface for mesh databases aimed exclusively at meshing operations [Steinbrenner et al. 2005]; results of such queries in the UGC interface are explicitly expressed as integer indices into data arrays, with obvious implications for how implementations of that interface must store data. The low-level UGC interface is similar in scope to our API, although we have deliberately been more general in providing support for functionality required by solvers and in emphasizing data structure neutrality.

In addition, several efforts have been made to define common interfaces to mesh data in the context of writing meshes to disk files. Two examples are the HDF Mesh API [HDF5 2008; 2007] and the CFD General Notation System (CGNS) [CFD General Notation System 2004; Legensky et al. 2002]. These efforts are similar in spirit, though they are either not complete enough (e.g. provide no mechanism to annotate mesh with other data) or address mesh data with a different level of abstraction than that chosen in our work.

1.1 A Simple Use Case for a Mesh Component

As an example of how a typical scientific computing application might benefit from using a mesh component, let us consider a finite element solver (FESolve) for some partial differential equation, and how this application might evolve over time.[1] Let us assume that when first developed, FESolve is a simple finite element solver, using linear elements. At run time, FESolve loads a mesh from a file and does some pre-processing of the mesh to compute geometric quantities (such as integration points and weights) and perhaps to compute some mesh topological relationships that weren't in the file. Then, FESolve iterates over the elements in the mesh, computing the residual and the stiffness matrix for each, and assembling these into a global linear system. This system is solved, and the solution is updated at every node. This iteration process may be repeated several times, e.g., for

[1]While different applications will surely have different requirements for interacting with unstructured mesh data, many, if not most, applications will follow roughly this same outline.

time-dependent or non-linear problems.

After FESolve has been in use for some time, its developers decide that mesh adaptation is required to improve solution accuracy and/or efficiency. With current approaches to developing mesh infrastructure software, they have two fundamentally different choices. One choice is to select some existing mesh adaptation code written by some other researcher(s) and integrate it with FESolve by resolving whatever impedance mismatch may exist. In many cases, this will require replacing the entire mesh database and infrastructure in FESolve with new software infrastructure from the mesh adaptation code, including updating FESolve to access data in a totally different way. The other choice is to ignore all existing mesh adaptation implementations and develop, from scratch, an implementation that is specifically tailored to fit into FESolve's current architecture. Of course, there are hybrid solutions which combine these two approaches.

A standard mesh component provides a third, less painful way to make this transition. Let us assume that there exists a stand-alone service that provides key mesh adaptation operations such as element division and coarsening. A mesh component interface can serve as the intermediary between the provider of mesh data (in this case, FESolve) and users of mesh data (in this case, the mesh adaptation service). The interface specifies a set of fundamental mesh query and manipulation operations. In essence, a mesh component interface proclaims "If you are going to ask me about a mesh, these are the questions you can ask and this is how you ask them." or "If you are going to operate on a mesh, these are the operations you can perform and this how you perform them." The component's data model specifies how mesh data is encapsulated.

When using a standard mesh component and a compliant adaptation service, the developers of FESolve are now required only to provide implementations of the component functionality used by the adaptation code. That is, if the mesh adaptation code uses only a handful of the queries and operations in the mesh component interface, then only this handful of functions needs to be added to FESolve. Once done, FESolve's data, in its own internal data structures, can be used directly by the mesh adaptation code without further integration. As a bonus, in implementing part of the mesh component interface, the FESolve development team will have done some of the work required to integrate other useful advanced capabilities available through the mesh component.

1.2 The ITAPS Mesh Component

In this paper, we will describe a newly developed component intended to provide support for the mesh access and manipulation requirements of practical, large-scale scientific computing applications. This component, developed as part of a larger project by the Interoperable Tools for Advanced Petascale Simulation (ITAPS) center to develop interoperable software tools for meshes, domain geometry, and solution representation [Chand et al. 2008], is called iMesh. Note the words "support for": the iMesh component is not intended to be a general interface to all possible meshing operations, but rather, to define the operations required at a mesh database level so that high-level operations — including mesh generation, mesh improvement, mesh adaptation, parallel partitioning, load balancing, and design optimization — can be implemented as *services* that store and manipulate mesh data by using the iMesh component and mesh databases that implement the component's functionality. To be genuinely useful to real applications and real application developers, the component must be

—general purpose: most common mesh operations must be implementable based on the iMesh component,

—efficient: data access using the iMesh component and its implementations must not come at too high a cost in overhead,

—flexible: different applications may want to use different approaches for the same task, and

—interoperable: implementations of the component must be truly interchangeable, and services designed to use the component should work on a plug and play basis, regardless of data structures and programming language.

Section 2 describes the design principles we followed to ensure that the iMesh component met these goals. We first defined a data model (see Section 3): meshing operations require information about mesh entities (like vertices, triangular faces, and hexahedral regions), collections of entities, and meta-data associated with mesh entities. Using that data model, we then defined an API that would support general meshing and mesh-related solver operations (see Section 4). In addition to defining the iMesh component interface, we have also developed implementations of it based on existing mesh databases and used these implementations for various meshing and PDE solution tasks; several examples will be given in Section 5. The paper will conclude with discussion of lessons learned from developing this component, of the current status of software using the iMesh component, and of future prospects for extension and application of the iMesh component.

2. DESIGN PRINCIPLES

In Section 1.2, we summarized our goals for the iMesh component. As design of the component interface continued, we found that several principles recurred frequently in guiding our design decisions as we worked towards those goals. Specifically, we found that we made decisions to produce an interface that was:

Comprehensive. Clearly, a minimal requirement is that most typical mesh operations must be possible, either intrinsically through the iMesh component API or by building on it.

Run-time efficiency. For the iMesh component to be useful for applications, it must have low overhead. Specifically, the component interface must be designed so that an iMesh implementation can provide data access and manipulation nearly as rapidly as native access to the same mesh database. An example of the application of this principle in the iMesh component interface are the availability of both single-entity and array-of-entities access to mesh data, either of which may be more efficient depending on the circumstances.

Ease of use. To lower the barrier for adoption of the interface, it must be relatively easy for programmers to use. This implies the interface must be relatively compact but also provide direct access to commonly used constructs, even at the expense of additional functions in the interface. For example, we recognize that certain types of metadata – specifically, double, integer, and entity handle metadata – will be very common and more easily handled both by iMesh implementations and applications if there are specific functions for these types. However, to preserve flexibility in such cases, we also provide general access mechanisms; for the metadata example, generic data is described using byte strings. Contrariwise, where this can be done without loss of functionality, we prefer to use a single, more general function rather than a collection of specific functions to reduce the number of functions programmers must learn and use; for example, all requests for entities adjacent to a given entity use the same function, rather than having separate functions for each possible adjacency.

Flexibility. We recognize that different applications may choose to express the same semantic content in different ways. Where feasible, the iMesh interface supports this. For example, one application may choose to represent boundary condition data by metadata attached to particular mesh entities; another may represent the same information by collecting those entities into a set and annotating the set instead. As another example, some applications may choose to access data entity by entity while others may prefer array access to data.

Extensibility. We have designed the interface to allow extensions to the low-level mesh access functionality that the interface defines. For example, ongoing work for a parallel extension to the iMesh interface leverages serial iMesh functionality for parallel usage.

Interoperability. In the long-term, success of the iMesh component will depend on how well the component truly supports interoperability. This is the key to being able to leverage the effort in development of both implementations and services as well as conversion of applications to use the interface. Interoperability, in turn, requires not only the use of a standard interface, but also data structure and programming language neutrality. Also, interoperability can be enhanced by eliminating gray areas, where component behavior is implementation-dependent.

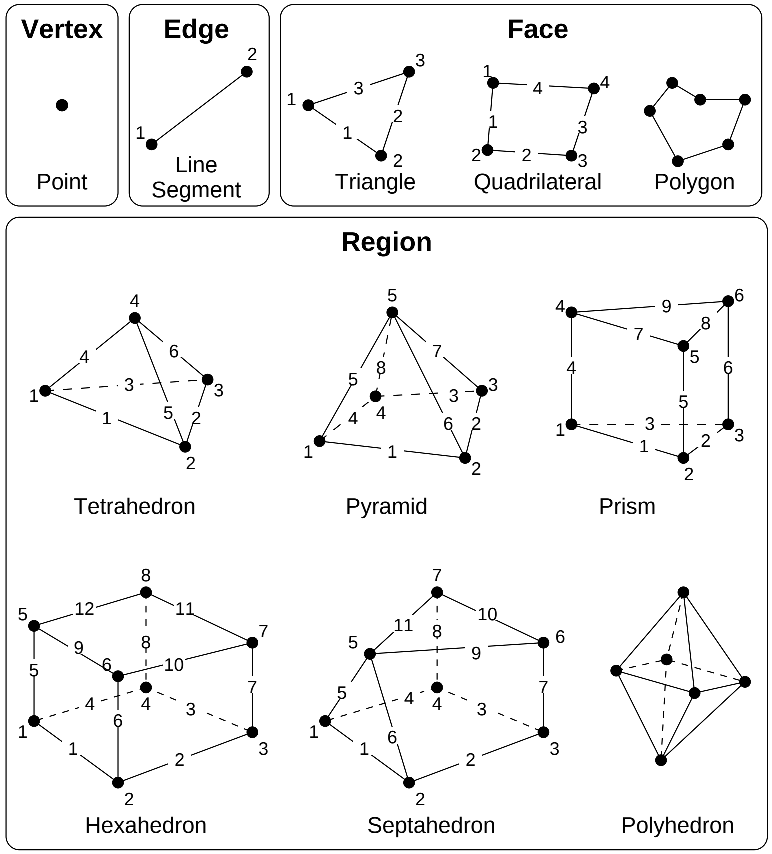
3. DATA MODEL

In the iMesh data model, all mesh primitives — vertices (0D), edges (1D), faces (2D), and regions (3D) — are referred to as *entities*. *Entity sets* are collections of mesh entities and other sets.. All topological and geometric mesh data,[2] as well as all other entity sets, are contained in a *root entity set*. To provide a scope for mesh data and to allow representation of multiple meshes, each root set is treated by the iMesh data model as an *instance*, which is analogous to a C++ object, though it need not be implemented this way (in this analogy, the iMesh interface definition is, loosely, a C++ class). In many implementations, the instance will be a database or collection of containers storing all of the mesh entities, with other entity sets containing handles for these entities rather than copies of all entity data. Any iMesh data object — an entity or any entity set including the root set — can have one or more *tags* associated with it, so that arbitrary data can be attached to the object. To preserve data structure neutrality, all iMesh data objects are identified by opaque handles. The interface makes no assumptions about the way these handles represent data; in particular, pointer and integer handles are treated identically in the interface and have been used in implementations.

3.1 Mesh Entities

All the primitive constituents of a mesh are defined by the iMesh data model as *entities*. iMesh entities are distinguished by their entity *type* (vertex, edge, face, or region: effectively, their topological dimension) and *topology* (for example, triangle, quadrilateral, or

[2] *Geometric mesh data* is geometric data required to define shapes of mesh entities. This is distinct from *geometric model data*, which defines the shape of the problem domain.

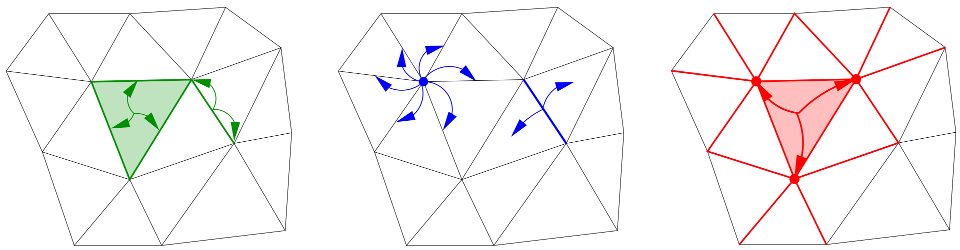


Entity	Canonical Ordering of Faces					
	1	2	3	4	5	6
Tetrahedron	△124	△234	△314	△132	—	—
Pyramid	△125	△235	△345	△415	□4321	—
Prism	□1254	□2365	□3146	△132	△456	—
Hexahedron	□1265	□2376	□3487	□4158	□4321	□5678
Septahedron	△125	□2365	□3476	□4157	□4321	△567

Fig. 1: Entities supported by the iMesh component. Canonical edge ordering is indicated in the sketch; canonical face ordering is given in the table. Polygons and polyhedra intrinsically have no canonical ordering.

tetrahedron). Each topology has a unique entity type associated with it. Examples of entities include vertices, edges, triangular or quadrilateral faces in 2D or 3D, and tetrahedral or hexahedral regions in 3D; a complete catalog of entities supported by iMesh is shown in Figure 1. Higher-dimensional entities are defined by lower-dimensional entities using a canonical ordering.

Adjacencies describe how mesh entities connect to each other. For an entity of dimension d, a first-order adjacency request returns all of the mesh entities of dimension q which are on the closure of the entity for downward adjacency ($d > q$), or for which the entity is part of the closure for upward adjacency ($d < q$), as shown in Figure 2(a) and (b). For an entity of dimension d, second-order adjacencies describe all of the mesh entities



(a) Downward adjacency; edges adjacent to a face, vertices adjacent to an edge.

(b) Upward adjacency: edges adjacent to a vertex, faces adjacent to an edge.

(c) Second adjacency; red edges are adjacent to vertices adjacent to the red face.

Fig. 2: Examples of adjacency relationships between mesh entities.

of dimension q that share any adjacent entities of dimension b, where $d \neq b$ and $b \neq q$. Second-order adjacencies can be derived from first-order adjacencies. Note that, in the iMesh data model, requests such as all vertices that are neighbors to a given vertex are requests for second-order adjacencies. Figure 2(c) highlights all edges adjacent to vertices adjacent to the shaded face.

3.2 Entity Sets

The iMesh data model allows arbitrary groupings of entities, called *entity sets*. Each entity set may be a true set (in the set theoretic sense) or it may be a (possibly non-unique) ordered list of entities; in the latter case, entities are retrieved in the order in which they were added to the entity set. An entity set may or may not be a simply-connected computational mesh; entity sets that *are* simple meshes have obvious application in multiblock and multigrid contexts, for instance. Entity sets (other than the root set) are populated by addition or removal of entities from the set. In addition, set Boolean operations — subtraction, intersection, and union — on entity sets are also supported.

Two primary relationships among entity sets are supported. First, entity sets may contain one or more entity sets (by definition, all entity sets belong to the root set). An entity set contained in another may be either a subset or an element (each in the set theoretic sense) of that entity set. The choice between these two interpretations is left to the application; the iMesh component does not impose either interpretation. Set contents can be queried recursively or non-recursively; in the former case, if entity set A is contained in entity set B, a request for the contents of B will include the entities in A (and the entities in sets contained in A). Second, parent/child relationships between entity sets are used to represent logical relationships between sets, including multigrid and adaptive mesh sequences. These logical relationships naturally form a directed, acyclic graph.

Examples of entity sets include the ordered list of vertices bounding a geometric face, the set of all mesh faces that lie on that geometric face, the set of regions assigned to a single processor by mesh partitioning, and the set of all entities in a given level of a multigrid mesh sequence.

For use with most solution applications, information in the root set or one or more of its constituent entity sets is typically a valid mesh for some scientific computing task, examples of which include:

—A non-overlapping, connected set of iMesh entities; for example, the structured and unstructured meshes commonly used in finite element simulations (*simple mesh*).

—Overlapping grids in which a collection of simple meshes are used to represent some portion of the computational domain, including chimera, multiblock, and multigrid meshes (*multiple mesh*). The interfaces presented here handle these mesh types in a general way; higher-level services may be added later to support specific functionalities needed by these meshes. In this case, each of the simple meshes is a valid computational mesh, stored as an entity set.

—Adaptive meshes in which all entities in a sequence of refined (simple or multiple) meshes are retained in the root set. The most highly refined adaptation level typically comprises a simple or multiple mesh. Typically, different levels of mesh adaptation will be represented by different entity sets, with many of the entities shared by multiple entity sets.

—Smooth particle hydrodynamic (SPH) meshes, which consist of a collection of iMesh vertices with no connectivity or adjacency information.

Meshing applications will typically have a valid computational mesh as their end product, though during processing the mesh database will often not be in this state.

3.3 Tags

Tags are used as containers for user-defined data that can be attached to iMesh entities and entity sets. Different values of a particular tag can be associated with different entities or sets; for instance, a boundary condition tag will have different values for an inflow boundary than for a no-slip wall, and no value at all for faces in the interior of the mesh. In the general case, iMesh tags do not have a predefined type and allow the user to attach arbitrary data to mesh entities; this data is stored and retrieved by implementations as a byte pattern. To improve performance and ease of use, we support three specialized tag types: integers, doubles, and entity handles. These typed tags enable an iMesh implementation to correctly save and restore tag data when a mesh is written to a file.

4. INTERFACE FUNCTIONALITY

The iMesh interface supports a variety of commonly needed functionalities for mesh and entity query, mesh modification, entity set operations, and tags. All data passed through the interface is in the form of opaque handles to objects defined in the data model. In this section we describe the functionality available through the iMesh interface.[3] For a reference implementation and simple usage examples, see the ITAPS web site [ITAPS Software Webpage 2007].

4.1 Global Queries

Global query functions can be categorized into two groups: 1) *database functions*, that manipulate the properties of the database as a whole and 2) *set query functions*, that query

[3]Note that these descriptions do not include detailed syntax, which can be found in the interface user guide [Chand et al. 2007a; 2007b]. Also, note that all function names in the interface are prepended by iMesh_; this prefix is omitted in the tables in this paper for compactness.

Table I: Functions for Global Queries. (All function names are prepended with iMesh_.)

Function	Description
newMesh	Creates a new, empty mesh instance
dtor	Destroys a mesh instance
load	Loads mesh data from file into entity set
save	Saves data from entity set to file
getRootSet	Returns handle for the root set
getGeometricDim	Returns geometric dimension of mesh
setGeometricDim	Sets geometric dimension of mesh (must not contain data yet)
getDfltStorage	Tells whether implementation prefers blocked or interleaved coordinate data
getAdjTable	Returns table indicating availability and cost of entity adjacency data
setAdjTable	Specifies requirements for entity adjacencies and iterators
areEHValid	Returns true if EH remain unchanged since last user-requested status reset
getNumOfType	Returns number of entities of type in ES
getNumOfTopo	Returns number of entities of topo in ES
getEntities	Returns all entities in ES of the given type and topology
getVtxArrCoords	For all input vertex handles, return coords; storage order can be user-specified.
getAdjEntIndices	Given ES and optionally a type or topology, return: EH's in ES of the specified type or topology; EH's adjacent to those entities with a specified type, as a list of unique handles; and for each entity in the first list, the adjacent entities specified as indices into the second list.

the contents of entity sets as a whole; these functions require an entity set argument, which may be the root set. These functions are summarized in Table I.

Database functions include functions to create and destroy mesh instances; note that the create function only sets up data structures for the mesh instance, which must be filled by reading data from a file or by creating a mesh entity by entity. The load and save functions read and write mesh information from files; file format and read/write options are implementation dependent. As mesh data is loaded, entities are stored in the root set, and can optionally be placed into a subsidiary entity set as well. iMesh implementations must be able to provide coordinate information in both blocked (xxx...yyy...zzz...) and interleaved (xyzxyzxyz...) formats; an application can query the implementation to determine the implementation's preferred storage order.

For a particular implementation, not all first-order adjacencies are necessarily available. For instance, in a classic finite element element-node connectivity storage, requests for faces or edges adjacent to an entity may return nothing, because the implementation has no stored data to return. For first-order adjacencies that are available in the implementation, the implementation may store the adjacency information directly, or compute adjacencies by either a local traversal of the entity's neighborhood or by global traversal of the entity set. Each iMesh implementation must provide information about the availability and relative cost of first-order adjacency queries. Also, a service or application may specify which adjacencies it requires and what entity types it will iterate over; this information, which can be updated by the service or application as its needs change, can be used by implementations to optimize internal storage for minimum memory use and efficient data retrieval.

Set query functions allow an application to retrieve information about entities in a set. The entity set may be the root set, which will return selected contents of the entire database, or may be any subsidiary entity set. For example, functions exist to request the number of

Table II: Functions for Single Entity Queries. (All function names are prepended with iMesh_.)

Function	Description
initEntIter	Create an iterator to traverse entities of type and topo in ES; return true if any entities exist
getNextEntIter	Return true and a handle to next entity if there is one; false otherwise
resetEntIter	Reset iterator to restart traverse from the first entity
endEntIter	Destroy iterator
getEntType	Return type of entity
getEntTopo	Return topology of entity
getVtxCoord	Return coordinates of a vertex
getEntAdj	Return entities of given type adjacent to EH
getEnt2ndAdj	Return entities of given type adjacent to entities of a second type adjacent to EH

Table III: Functions for Block Entity Queries. (All function names are prepended with iMesh_.)

Function	Description
initEntArrIter	Create a block iterator to traverse entities of type and topo in ES
getNextEntArrIter	Return true and a block of handles if there are any; false otherwise
resetEntArrIter	Reset block iterator to restart traverse from the first entity
endEntArrIter	Destroy block iterator
getEntArrType	Return type of each entity
getEntArrTopo	Return topology of each entity
getEntArrAdj	Return entities of type adjacent to each EH
getEntArr2ndAdj	Return entities of given type adjacent to entities of a second type adjacent to each EH

mesh entities of a given type or topology; the types and topologies are defined as enumerations. Applications can request handles for all entities of a given type or topology or handles for entities of a given type adjacent to all entities of a given type or topology. Also, vertex coordinates are available in either blocked or interleaved order. Coordinate requests can be made for the arrays of vertex handles returned by an adjacency call. Finally, for entities of a given type and topology, their adjacent entities of a given type can be returned, along with an array of compressed sparse row style indices into the global vertex coordinate array can be obtained for both entity and adjacent entity requests.

4.2 Entity- and Array-Based Query

The global queries described in the previous section are used to retrieve information about all entities in an entity set. While this is certainly a practical alternative for some types of problems and for small problem size, larger problems or situations involving mesh modification require access to single entities or to blocks of entities. The iMesh interface supports traversal and query functions for single entities and for blocks of entities; the query functions supported are entity type and topology, vertex coordinates, and entity adjacencies. Blocks of data are passed through the interface using arrays of entity handles. Tables II and III summarize these functions.

4.3 Mesh Modification

The iMesh interface supports mesh modification by providing a minimal set of operators for low-level modification; both single entity (see Table IV) and block versions (see Ta-

Table IV: Functions for Single Entity Mesh Modification. (All function names are prepended with iMesh_.)

Function	Description
createVtx	Create vertex at given location
setVtxCoords	Changes coordinates of existing vertex
createEnt	Create entity of given topology from lower-dimensional entities; return entity handle and creation status
deleteEnt	Delete EH from the mesh

Table V: Functions for Block Mesh Modification. (All function names are prepended with iMesh_.)

Function	Description
createVtxArr	Create vertices at given location
setVtxArrCoords	Changes coordinates of existing vertices
createEntArr	Create entities of given topology from lower-dimensional entities; return entity handle and status
deleteEntArr	Delete each EH from the mesh

ble V) of these operators are provided. High-level functionality, including mesh generation, quality assessment, and validity checking, can in principle be built from these operators, although in practice such functionality is more likely to be provided using intermediate-level services that perform complete unit operations, including vertex insertion and deletion with topology updates, edge and face swapping, and vertex smoothing.

Geometry modification is achieved through functions that change vertex locations. Vertex locations are set at creation, and can be changed as required, for instance, by mesh smoothing or other vertex movement algorithms.

Topology modification is achieved through the creation and deletion of mesh entities. Creation of higher-dimensional entities requires specification, in canonical order, of an appropriate collection of lower-dimensional entities. For instance, a tetrahedron can be created using four vertices, six edges or four faces, but not from combinations of these. Upon creation, adjacency information properly connecting the new entity to its closure is set up by the implementation. Some implementations may allow the creation of duplicate entities (for example, two edges connecting the same two vertices), while others will respond to such a creation request by returning a copy of the already-existing entity.

Deletion of existing entities is typically done from highest to lowest dimension. The iMesh interface also allows the deletion of an entity with existing upward adjacencies (for instance, an edge that is still in use by one or more faces or regions); in this case, downward adjacency requests may be nonsensical.

4.4 Entity Sets

Entity set functionality in the iMesh interface is divided into three parts: basic set functionality, hierarchical set relations, and set Boolean operations.

Basic set functionality, summarized in Table VI, includes creating and destroying entity sets; adding and removing entities and sets; and several entity set specific query functions.[4] Entity sets can be either ordered and non-unique, or unordered and unique; an ordered set guarantees that set query results (including traversal) will always be given in the order in

[4]Note that the global mesh query functions (Section 4.1) and traversal functions (Section 4.2) defined above can be used with the root set or any other entity set as their first argument.

Table VI: Functions for Basic Entity Set Functionality. (All function names are prepended with iMesh_.)

Function	Description
createEntSet	Creates a new entity set (ordered and non-unique if isList is true)
destroyEntSet	Destroys existing entity set
isList	Return true if the set is ordered and non-unique
getNumEntSets	Returns number of entity sets contained in SH
getEntSets	Returns entity sets contained in SH
addEntSet	Adds entity set SH1 as a member of SH2
rmvEntSet	Removes entity set SH1 as a member of SH2
isEntSetContained	Returns true if SH2 is a member of SH1
addEntToSet	Add entity EH to set SH
rmvEntFromSet	Remove entity EH from set SH
addEntArrToSet	Add array of entities to set SH
rmvEntArrFromSet	Remove array of entities from set SH
isEntContained	Returns true if EH is a member of SH
isEntArrContained	Check an array of entities for membership in SH

Table VII: Functions for Entity Set Relationships. (All function names are prepended with iMesh_.)

Function	Description
addPrntChld	Create a parent (SH1) to child (SH2) relationship
rmvPrntChld	Remove a parent (SH1) to child (SH2) relationship
isChildOf	Return true if SH2 is a child of SH1
getNumChld	Return number of children of SH
getChldn	Return children of SH
getNumPrnt	Return number of parents of SH
getPrnts	Return parents of SH

Table VIII: Functions for Entity Set Boolean Operations. (All function names are prepended with iMesh_.)

Function	Description
subtract	Return set difference SH1-SH2 in SH
intersect	Return set intersection of SH1 and SH2 in SH
unite	Return set union of SH1 and SH2 in SH

which entities were added to the set. The ordered/unordered status of an entity set must be specified when the set is created and can be queried.

Entity sets are created empty. Entities can be added to or removed from the set individually or in blocks; for ordered sets, the last of a number of duplicate entries will be the first to be deleted. Also, entity sets can be added to or removed from each other; note that, because all entities and sets are automatically contained in the root set from creation, calls that would add or remove an entity or set from the root set are not permitted. An entity set can also be queried to determine the number and handles of sets that it contains, and to determine whether a given entity or set belongs to that set.

Hierarchical relationships between entity sets are intended to describe, for example, multilevel meshes and mesh refinement hierarchies. The directional relationships implied here are labeled as parent-child relationships in the iMesh interface. Functions are provided to add, remove, count, and identify parents and children and to determine if one set is a child of another; see Table VII.

Set Boolean operations — intersection, union, and subtraction — are also defined by the iMesh interface; these functions are summarized in Table VIII. The definitions are intended to be compatible with their C++ standard template library (STL) counterparts, both for semantic clarity and so that STL algorithms can be used by implementations where appropriate. All set Boolean operations apply not only to *entity* members of the set, but also to *set* members. Note that set hierarchical relationships are not included: the set resulting from a set Boolean operation on sets with hierarchical relationships will *not* have any hierarchical relationships defined for it, regardless of the input data. For instance, if one were to take the intersection of two directionally-coarsened meshes (stored as sets) with the same parent mesh (also a set) in a multigrid hierarchy, there is no reason to expect that the resulting set will necessarily be placed in the multigrid hierarchy at all. On the other hand, if both of those directionally-coarsened meshes contain a set of boundary faces, then their intersection will contain that set as well.

While set Boolean operations are completely unambiguous for unordered entity sets, ordered sets make things more complicated. For operations in which one set is ordered and one unordered, the result set is unordered; its contents are the same as if an unordered set were created with the (unique) contents of the ordered set and the operation were then performed. In the case of two ordered sets, the iMesh specification tries to follow the spirit of the STL definition, with complications related to the possibility of multiple copies of a given entity handle in each set. We recognize that these rules are somewhat arbitrary, but have been unable to find a more systematic way of defining these operations for ordered sets. In the following discussion, assume that a given entity handle appears m times in the first set and n times in the second set.

—For intersection of two ordered sets, the output set will contain $\min(m,n)$ copies of the entity handle. These will appear in the same order as in the first input set, with the first copies of the handle surviving. For example, intersection of the two sets $A = \{abacdbca\}$ and $B = \{dadbac\}$ will result in $A \bigcap B = \{abacd\}$.

—Union of two ordered sets is easy: the output set is a concatenation of the input sets: $A \bigcup B = \{abacdbcadadbac\}$.

—Subtraction of two ordered sets results in a set containing $\max(m-n,0)$ copies of an entity handle. These will appear in the same order as in the first input set, with the first copies of the handle surviving. For example, $A - B = \{abc\}$.

Regardless of whether the entity members of an entity set are ordered or unordered, the set members are always unordered and unique, with correspondingly simple semantics for Boolean operations.

4.5 Tags

Tags are used to associate application-dependent data with a mesh, entity, or entity set. Basic tag functionality defined in the iMesh interface is summarized in Table IX, while functionality for setting, getting, and removing tag data is summarized in Table X.

When creating a tag, the application must provide its data type and size, as well as a unique name. For generic tag data, the tag size specifies how many bytes of data to store; for other cases, the size tells how many values of that data type will be stored. The implementation is expected to manage the memory needed to store tag data. The name string and data size can be retrieved based on the tag's handle, and the tag handle can be

Table IX: Basic Tag Functions. (All function names are prepended with iMesh_.)

Name	Description
createTag	Creates a new tag of the given type and number of values
destroyTag	Destroys the tag if no entity is using it or if force is true
getTagName	Returns tag ID string
getTagSizeValues	Returns tag size in number of values
getTagSizeBytes	Returns tag size in number of bytes
getTagHandle	Return tag with given ID string, if it exists
getTagType	Return data type of this tag
getAllTags	Return handles of all tags associated with entity EH
getAllEntSetTags	Return handles of all tags associated with entity set SH

Table X: Setting, Getting, and Removing Tag Data. (All function names are prepended with iMesh_.)

Function	Description
setData	The value in tag TH for entity EH is set to the first tagValSize bytes of the array<char> tagVal
setArrData	The value in tag TH for entities in EHarray[i] is set using data in the array<char> tagValArray and the tag size
setEntSetData	The value in tag TH for entity set SH is set to the first tagValSize bytes of the array<char> tagVal
set[Int,Dbl,EH]Data	The value in tag TH for entity EH is set to the int, double, or entity handle in tagVal; array and entity set versions also exist.
getData	Return the value of tag TH for entity EH
getArrData	Retrieve the value of tag TH for all entities in EH array, with data returned as an array of tagVal's
getEntSetData	Return the value of tag TH for entity EH
get[Int,Dbl,EH]Data	Return the value of tag TH for entity EH; array and entity set versions also exist.
rmvTag	Remove tag TH from entity EH
rmvArrTag	Remove tag TH from all entities in EH array
rmvEntSetTag	Remove tag TH from entity set SH

found from its name. Also, all tags associated with a particular entity can be retrieved; this can be particularly useful in saving or copying a mesh.

Initially, a tag is not associated with any entity or entity set, and no tag values exist; association is made explicitly by setting data for a tag-entity pair. Tag data can be set for single entities, arrays of entities (each with its own value), or for entity sets. In each of these cases, separate functions exist for setting generic tag data and type-specific data. Analogous data retrieval functions exist for each of these cases.

When an entity or set no longer needs to be associated with a tag — for instance, a vertex was tagged for smoothing and the smoothing operation for that vertex is complete — the tag can be removed from that entity without affecting other entities associated with the tag. When a tag is no longer needed at all — for instance, when all vertices have been smoothed — the tag can be destroyed through one of two variant mechanisms. First, an application can remove this tag from all tagged entities, and then request destruction of the tag. Simpler for the application is forced destruction, in which the tag is destroyed even though the tag is still associated with mesh entities, and all tag values and associations are deleted. Some implementations may not support forced destruction.

Table XI: Error Handling Functionality. (All function names are prepended with iMesh_.)

Name	Description
getDescription	Retrieves error description

4.6 Error Handling

Like any API, the iMesh interface is vulnerable to errors, either through incorrect input or through internal failure within an implementation. For instance, it is an error for an application to request entities with conflicting types and topologies. Also, an error in the implementation occurs when memory for a new object cannot be allocated. The iMesh interface defines a number of standard error conditions which could occur in iMesh functions, either because of illegal input or internal implementation errors; each of these error conditions has an accompanying description, which can be retrieved by calling iMesh_getDescription, summarized in Table XI.

4.7 Compliance Testing

To ensure consistency between implementations and to assist users developing partial implementations based on their own mesh data structures, we have developed a comprehensive compliance test suite for the iMesh interface. When testing a full implementation of the interface, the test suite uses the iMesh implementation to read a mesh file, then tests each interface function. These tests are typically done by comparing information retrieved in multiple ways — for instance, retrieving coordinate information in both blocked and interleaved order, or retrieving adjacency information entity-by-entity or for all entities of a given type. The set and tag functions can be easily tested by creating sets or tags in the test code and querying the new sets and tags to verify their correctness. We are currently working on a function-level compliance testing, so that users wishing to use a single iMesh-based service can implement and test only the functions required for that service. This fine-grained testing is much more difficult, because consistency between different calls can no longer be relied on. The combination of these two test suites will ensure that different iMesh implementations have the same behavior, and that applications can rely on correct interaction with iMesh services.

4.8 Fortran Compatibility

For compatibility with the Fortran convention that functions returning values do not modify their arguments, no iMesh function returns a value. That is, all iMesh functions are C void functions or Fortran subroutines. Also, string arguments in the C API have an accompanying argument giving their length; these string length arguments are added at the end of the argument list in the order the strings appear. Fortran77 and Fortran90/95 compilers must support the pass-by-value extension to be compatible with the iMesh API. Fortran 2003 has C interoperability features that greatly simply matters; we provide a Fortran 2003 module definition and examples online [ITAPS Software Webpage 2007].

5. USAGE EXAMPLES

In this section, we provide several examples of using the iMesh component, including finite element simulation, mesh modification, mesh partitioning, and visualization. Each of these services has been demonstrated to work with multiple implementations of the iMesh component, and — where efficiency data are available — the overhead of using the iMesh

API rather than a native implementation is quite small. In addition to these examples of direct iMesh usage, members of our consortium are collaborating with applications researchers to introduce ITAPS software tools into applications in accelerator design, nuclear fusion, groundwater simulation, combustion, and computational biology; these efforts are not described in this paper.

5.1 Existing iMesh Implementations

Before discussing applications of the iMesh interface, we will summarize the status of the existing iMesh implementations. Our consortium has produced a complete reference implementation of the iMesh interface as well as four complete implementations based on our pre-existing mesh databases, all of which are available directly through our website [ITAPS Software Webpage 2007]; most also have their own websites. Each of the five supports all standard finite element topologies — hexahedra, tetrahedra, prisms, pyramids, triangles, and quadrilaterals. Each has its own particular strengths and areas of most frequent application.

—The reference implementation (RefImpl) is intended as a basic mesh database with full support for all iMesh functionality. Users looking for a testbed for experimenting with iMesh or for implementing meshing algorithms without the difficulties of first writing a mesh database will find this implementation of particular interest.

—The Flexible Mesh DataBase (FMDB) [Remacle and Shephard 2003] is designed especially to handle adaptively changing mesh data, including flexible storage of adjacency information. Application usage of FMDB includes computational fluid dynamics (CFD), fusion, and accelerator simulations.

—The Mesh Oriented datABase (MOAB) [Tautges et al. 2004] is particularly efficient in its memory management. Application usage for MOAB includes nuclear reactor modeling, neutron transport, and accelerator design optimization.

—The Generation and Refinement of Unstructured Mixed-element Meshes in Parallel (GRUMMP) [Ollivier-Gooch 2005] toolkit is designed for triangular/tetrahedral mesh generation, improvement, and adaptation, and is particularly efficient in retrieving adjacency information. Application usage is primarily in CFD, especially aerodynamics and non-Newtonian fluid dynamics.

—The Pacific Northwest National Laboratory's NWGRID [Trease and Trease 2004] is intended for adaptive mesh refinement, especially for simplicial meshes. Application usage includes computational biology, CFD, solid mechanics, and subsurface transport modeling.

5.2 A Simple Finite Element Solver

To demonstrate the cost of using the iMesh interface in a typical computational science application, we developed a simple finite element application that solves a diffusion problem in two dimensions on the unit square:

$$\nabla(k\nabla u(x,y)) = f \tag{1}$$

$$u(x=0)=0 \quad u(x=1)=1 \quad u_x(y=0)=0 \quad u_x(y=1)=0. \tag{2}$$

The finite element solver uses linear triangular elements and exact integration rules. The finite element solver is written in C and uses PETSc to solve the linear systems.

Table XII: iMesh functions used in the simple finite element solver for different mesh data access

Array Access	Entity Iterator	Entity Array Iterator
getRootSet	getRootSet	getRootSet
getTagHandle	getTagHandle	getTagHandle
getVtxCoordIndex	initEntIter	initEntArrIter
getAllVtxCoords	getNextEntIter	getNextEntArrIter
getEntities	getEntAdj	getEntArrAdj
getIntArrData	getVtxCoord	getVtxArrCoords
getDblArrData	getIntData	getIntArrData
	getDblArrData	getDblArrData

We focus our attention on setting up the linear system and consider four different options for accessing the mesh data: 1) through array-based mechanisms defined in the iMesh interface, which should approximate the performance of a native implementation; 2) through entity iterators; and 3) through entity array iterators. Regardless of access method, we require for each vertex its coordinates; a global id and a boundary flag as stored attached to the vertices as tags. For elements, we require downward adjacency information (face to vertex) and store a global id and computed element area as tags. We make use of the iMesh functions given in Table XII. In all cases, we must obtain the root set from the iMesh instance and get the tag handles for the global ids, boundary flags and element areas. In the case of array access, we obtain a lists of all the vertex and face entities in the mesh and can obtain the tag data as arrays of size *num_vtx* or *num_elem*. We can obtain the vertex coordinate information and element connectivity information using these entity arrays or, as we did in this example, directly from the mesh data base. It is guaranteed by the iMesh interface that the information returned using these array-based calls will have a consistent ordering across all calls. The iMesh calls used for the entity and entity array iterators provide the same functionality either entity by entity or for arrays of entities. In each case, we initialize the iterator to return mesh faces and get entity information through the getNextEnt(Arr)Iter function. For each entity (array) returned, we obtain the downward vertex adjacency information, the vertex coordinates, and needed global id, boundary, and element area tag data.

This application has been timed with two iMesh implementations, GRUMMP and SimpleMesh, a small-scale test implementation developed at Lawrence Livermore; the application has also been tested successfully with other iMesh implementations, although timings are not reported here. We ran each case 40 times and report the average time required to set up the linear system in milliseconds, along with the percentage increase in cost compared to the use of problem-sized arrays, in Table XIII. In the case of the entity array iterator, we used array sizes of 1, 3, 5, 10 and 20. This is a small problem size; the total number of elements in the mesh is 6077, so the largest array iterator represents only about 0.3% of the total problem size. Not surprisingly, the array based access to the vertex and element information is the fastest. Entity iterators are perhaps the most natural to program, but result in the highest overhead costs due to the very large number of function calls $(10+3\cdot(n_e+n_e\cdot n_v)+4\cdot n_v)$, where n_e is the number of elements and n_v is the number of vertices; for the SimpleMesh implementation, the overhead is only 6.6%, but for the GRUMMP implementation it is a much higher 27.6%. The entity array iterator cases decrease in cost as the array size grows and number of function calls decreases; in this case, the total number of iMesh function calls is $10+6*n_e/|WS|+4*n_v/|WS|$, where $|WS|$ is the size of the work set; for both implementations, the overhead is reduced by at least a factor of two compared with entity iterators.

Table XIII: Timing results for the 2D linear finite element solver using the SimpleMesh implementation of the iMesh interface.

Case	SimpleMesh		GRUMMP	
	Time (ms)	$\frac{(T-T_{\text{array}})}{T_{\text{array}}} \times 100$	Time (ms)	$\frac{(T-T_{\text{array}})}{T_{\text{array}}} \times 100$
Array-based	81.8	—	86.7	—
Entity Iterator	87.2	6.6%	110.6	27.6%
Entity Array Iterator (1)	87.6	7.1%	109.0	25.8%
Entity Array Iterator (3)	86.2	6.7%	102.5	18.2%
Entity Array Iterator (5)	85.3	4.3%	99.0	14.1%
Entity Array Iterator (10)	85.4	4.5%	97.4	12.3%
Entity Array Iterator (20)	84.4	3.3%	95.9	10.6%

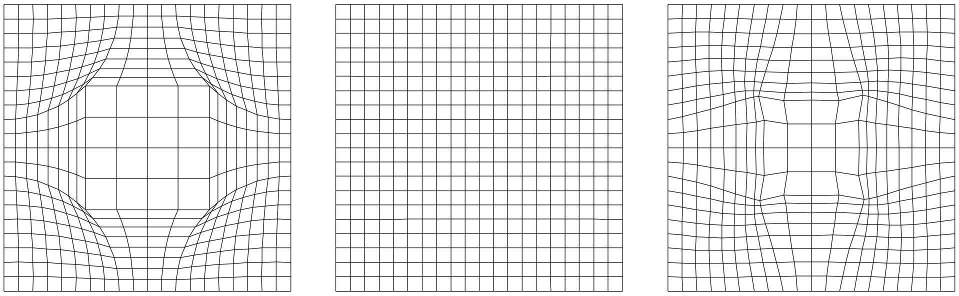
5.3 Mesh Quality Improvement via Vertex Movement

The MESh QUality Improvement Toolkit (Mesquite)[Brewer et al. 2003] improves the accuracy of mesh-based simulations through optimization of the mesh vertex locations. Mesquite can be used for element shape optimization, r-adaptivity, mesh alignment, etc., and has been tested with the MOAB, FMDB, GRUMMP and NWGRID iMesh implementations.

As input Mesquite requires an iMesh instance and entity set handle designating the subset of the mesh over which to perform the optimization. If the entity set handle is the root set, optimization is done for the entire mesh. Further, Mesquite expects an integer tag indicating whether the corresponding vertex may be moved during optimization. Generally, boundary vertices are marked as fixed or otherwise constrained to the computational domain boundary to ensure correct problem formulation. While there is some variation in iMesh functionality requirements in the different Mesquite solvers, all Mesquite optimization algorithms require iteration over elements and vertices contained in an entity set, element-vertex adjacency queries, entity set creation and modification,[5] vertex coordinate query and modification, and tag data query. These capabilities are sufficient to support Mesquite's global element shape optimizer; a sample input mesh is shown in Figure 3(a) with the corresponding output mesh in Figure 3(b). When optimizing a single vertex or subsets of mesh vertices, iMesh implementation must also efficiently determine the elements adjacent to a vertex. Output results were identical for both the global and Laplacian smoothers, and for data access using Mesquite's native mesh representation and via the iMesh interface.

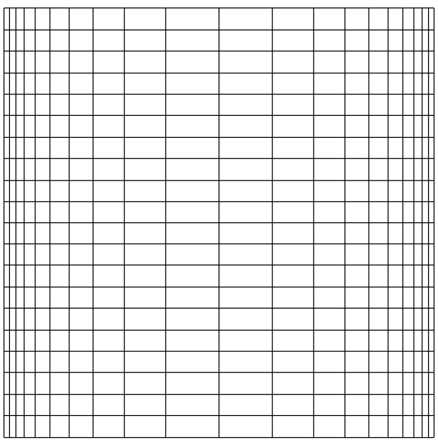
Mesquite is also capable of optimizing to obtain specific characteristics of the mesh on an element-by-element basis using target matrices. These pre-calculated target matrices are stored as iMesh tag data on the mesh elements and retrieved during optimization. For example, Figure 3(c) is the result of optimizing the same input mesh given previously, except that target matrices are used to preserve the size and aspect ratio of the elements. Another example is shown in Figure 4 in which element aspect ratio is preserved while

[5]This is an artifact of early versions of both Mesquite and the iMesh interface. The Mesquite-iMesh interaction code could be updated to remove the need for this capability.

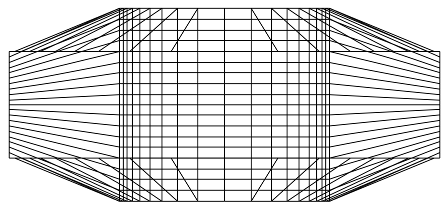


(a) Initial mesh (b) Optimized mesh (c) Optimized mesh using target matrix optimization

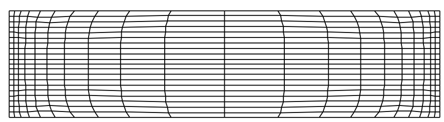
Fig. 3: Element shape optimization using Mesquite.



(a) Initial mesh



(b) Deformed mesh



(c) Optimized mesh

Fig. 4: Deforming boundary optimization using Mesquite.

Table XIV: CPU Time (seconds) for optimization of 40,000 element meshes.

Optimizer	Internal	iMesh	
		MOAB	GRUMMP
Global shape optimization	45.38	45.16	45.16
Laplacian smoother	111.60	472.65	—
Target matrix optimization	79.30	82.65	89.38
Deforming boundary	12.73	15.48	21.59

updating the mesh for a deforming mesh boundary. An initial anisotropic mesh, shown in Figure 4(a), is used to calculate the target matrices. Figure 4(b) shows the same mesh after boundary deformation, with some elements inverted due to the change in location of the boundary vertices. This mesh (with the stored target matrices) is the input to the Mesquite optimizer. The resulting mesh, with the element anisotropy preserved, is shown in Figure 4(c).

Table XV: Performance for the iMesh swapping service for a supersonic aircraft mesh (251,140 tetrahedra).

	Native (non-iMesh)	GRUMMP iMesh
Swaps	25,448	28,629
Rate ($\frac{1}{\text{sec}}$)	3,380	2,800
Memory (MB)	216 MB	292 MB

Table XIV shows the impact of the iMesh interface and implementation on optimizer performance.[6] Each row of the table corresponds to one of the examples above with the mesh interval size reduced by a factor of ten, resulting in meshes with 40,000 elements. The global shape optimization results demonstrate one of the advantages of using a mesh database library over a custom storage scheme. The more compact representation of data in the iMesh implementations results in a slight performance improvement over Mesquite's internal mesh representation. The Laplacian smoothing times emphasize the overhead of a standard interface and generalized mesh database. The smoothing calculation is trivial. The time spent in tens of millions of queries for small amounts of data (adjacencies, tag data, vertex coordinates, etc.) dominates the run time of the optimization. The latter two rows in Table XIV demonstrate the run time cost of accessing tag data. The time spent accessing other mesh data is the same as for the global shape optimization case. The difference in run time for each mesh database is entirely a function of the time spent querying target matrices stored in tag data.

5.4 Mesh Quality Improvement via Topology Optimization

Local mesh topology optimization can be a powerful tool for improving the quality of unstructured meshes; however, mesh topology modification — often referred to as swapping — is difficult enough to implement that an iMesh-based service that performs these operations would be useful for many applications. The classic face and edge swapping operations (see, for instance, [Freitag and Ollivier-Gooch 1997] for a description) have been implemented using the iMesh API [Ollivier-Gooch 2006].

The swapping service represents a worst-case scenario for efficiency tests for the iMesh interface, in that the service requires fine-grained access to and modification of the mesh database using the interface. As such, the swapping service makes a large number of calls through the interface, each returning a small amount of data. Specifically, the swapping service uses the iMesh entity iterators, adjacency queries, array-based vertex coordinate queries, checks for entity type and topology, and entity creation and deletion functions. Optionally, the swapping service can also be restricted to reconfigure only tetrahedra that are members of a given set, requiring the ability to query set membership and to assign new entities to sets. A second optional functionality is the ability to accept a tag and tag value to indicate which faces within a set should be considered for swapping.

The swapping service has been tested with three different iMesh implementations: GRUMMP, MOAB, and FMDB, and the results compared with an implementation of the same algorithms using the GRUMMP back-end (referred to as *native*). For testing purposes, we use a mesh for a supersonic aircraft initially containing 251,140 tetrahedra. Because of

[6]The iMesh implementation in GRUMMP does not yet support vertex-to-element adjacency queries for surface meshes, so it was not possible to run this Laplacian smoothing example with the GRUMMP iMesh implementation.

differences in the order in which faces are accessed, output meshes from the iMesh swapping service are not identical but we have confirmed elsewhere [Ollivier-Gooch 2006] that the meshes have statistically indistinguishable quality. Table XV compares the number of swaps performed, the swapping rate, and the memory used for the native swapping implementation and the swapping service using the GRUMMP iMesh implementation. The CPU time overhead for using the GRUMMP iMesh implementation rather than the native implementation is about 20% for this case; the 40% overhead in memory usage is required to support certain forms of entity creation that are not supported natively by the mesh database. Preliminary timing results for the MOAB and FMDB databases suggest that, for this service, good performance depends on careful attention to optimization of frequently-called iMesh functions, especially iterators and adjacency retrieval; in some cases, design decisions in the mesh database may also have a significant impact on performance.

5.5 A Partitioning Service

As a precursor to our ongoing work for a parallel extension to the iMesh interface, an iMesh-based service that performs partitioning would be useful. Partitioning distributes data over sets of processors and is needed by unstructured and/or adaptive parallel applications. Many of the partitioning methods in Zoltan [Boman et al. 2007] have been made available in a service that uses the iMesh API to access mesh data. The partitioners available can be grouped into three categories; simple partitioners for testing and demonstration, geometric or coordinate-based partitioners, and graph partitioning.

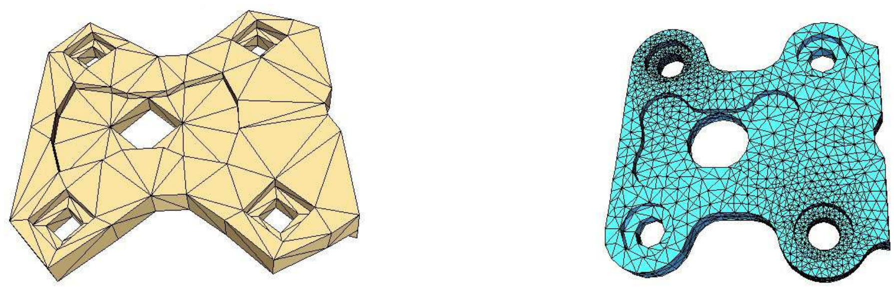
For the simple partitioners, the partitioning service uses the iMesh queries for entities and number of entities. The partition service can operate at the level of any mesh entity (i.e. vertex, edge, face, or region). The partitioning service uses both single-entity and array-of-entities access to mesh data. For the geometric partitioners, the partitioning service uses the iMesh single-entity adjacency queries and array-based vertex coordinate queries. For graph partitioning, the partitioning service uses the array-based adjacency queries.

The partition data is stored by both attaching an integer tag to each mesh entity and collecting entities into sets with integer tags. Any previous partition data is destroyed before new partition data is created. The partition service uses entity set query, deletion, and creation functions as well as the ability to assign new entities to sets and get, destroy, create, and set tag data.

The partitioning service has been tested and is interoperable with three mesh database implementations available through the iMesh C interface: MOAB, FMDB, and GRUMMP. Users need only link in the desired implementation; no other changes are necessary. A partitioning service interfacing directly to MOAB performs only slightly faster than the partitioning service interfacing to MOAB through iMesh. To partition a mesh with 1.4 million faces by faces using recursive coordinate bisection, the MOAB native implementation required 37.2 seconds, while using the ITAPS C interface to access the MOAB data structures required 38.2 seconds (2.5% overhead).

5.6 Visualization Using the iMesh Interface

Visualization and interactive manipulation of meshes as well as fields defined on meshes is important in many aspects of simulation software development. Towards this end, we have developed a VisIt [Childs et al. 2005] plugin that accesses mesh and solution data through an iMesh implementation. We have demonstrated that the current plugin is interoperable across three different iMesh implementations: GRUMMP, MOAB and FMDB. The plugin



(a) Before refinement (408 regions)

(b) After refinement (36,261 regions)

Fig. 5: An example of size field-based mesh adaptation.

uses array-based vertex coordinate queries. Solution data is retrieved using iMesh tag capabilities. In addition, the plugin uses recursive entity set queries to map an iMesh entity set hierarchy to a roughly equivalent VisIt construct called a *subset inclusion lattice*. This enables VisIt to provide intuitive GUI controls to users in terms of subsets that are characteristic to various stages of their design and analysis workflows. For example, users often need to focus their attention on a specific part in the original CAD model, a specific regime in the material model, or a specific discretization region in the numerical model. The ability for users to interactively visualize, query, calculate and otherwise analyze data in terms of characteristic subsets such as these both within and across each stage of a design and analysis workflow fundamentally enhances the flexibility of the analysis activities possible within the VisIt visualization tool.

5.7 Size Field-Based Mesh Adaptation

Adaptive methods are central to ensuring the accuracy and reliability of simulation results. One approach to supporting mesh adaptation is to provide a service that can take an existing mesh with a new mesh size field associated with it and create the desired adapted mesh by applying appropriate mesh modification operations. Such a service for anisotropic mesh adaptation has been under development of a number of years [Li et al. 2005]. To ensure the ability to deal with general curved geometries that can come from CAD systems, the service builds on a generalized interaction with the geometric model [Beall et al. 2004] and ensures the mesh can properly represent the domain of interest [Li et al. 2003]. This service has been used to construct adaptive simulation procedures by combining it with finite element and finite volume solvers, and associated error indicators. Since the mesh adaptation service works off a general anisotropic mesh size field, error indicators that have been used include various combinations of analytic fields, anisotropic *a posteriori* correction indicators and geometric approximation considerations [Shephard et al. 2005; Wan et al. 2005]. An example of a part before and after refinement using this approach is shown in Figure 5.

The current version of the mesh adaptation service builds on the FMDB mesh library that employs mesh topology like iMesh. Although it is possible to replace all FMDB calls with iMesh calls in the mesh adaptation service code (an activity planned for the future), the size of the code and the desire to apply the mesh adaptation to applications quickly prompted us to take an alternative initial approach. In this approach, meshes are accessed through the iMesh functions and loaded into the FMDB structures. The mesh adaptation process is carried out and the resulting mesh is then put back into iMesh form. This approach has the disadvantage that at the beginning and end of the mesh adaptation process there are two copies of the mesh. However, since the size of the mesh is typically small compared to the structures used during the implicit finite element and finite volume solvers being used to date, there have not been memory limitations introduced by this process.

6. DISCUSSION AND CONCLUSIONS

In this paper, we have described a new software component for mesh-based applications — both meshing and solver applications. We have described in detail the key features of this software component, called iMesh: its data model — which defines the types of data that the component works with — and its interface — which defines how applications can interact with mesh data.

Also, we have shown by example that iMesh component is flexible enough for a wide range of applications — including finite element solvers, mesh improvement and adaptation, partitioning, and visualization. Our experience with these examples shows that relatively complex mesh modification and solution requirements can be met by the interface, with low impact on efficiency. Specifically, for a simple finite element solver, overhead induced by using the iMesh interface is less than 10%, especially when data for multiple entities is retrieved through the mesh interface at once. For mesh smoothing, the overhead rate varied significantly from case to case, depending on the amount of work done by the smoothing code relative to the number of calls through the mesh interface. For mesh swapping, another fine-grained use case for the mesh component, overhead rates were about 20% compared with a native implementation of the same algorithms. Three higher-level services — mesh partitioning, visualization, and mesh adaptation — have also been tested across multiple iMesh implementations. In each case, the services have proved to be interoperable, and the overhead in using the iMesh interface is acceptable. Overall, our experience with these services confirms that relatively complex mesh operations can be performed correctly using the iMesh interface. Also, we have found clear examples of significant differences between mesh database designs in overall run time for a particular service.[7]

Several implementations of the iMesh component are currently available, as are the services described in this paper.[ITAPS Software Webpage 2007] An analogous software component for geometric query and manipulation for mesh-based applications has also been developed, and work is nearing completion on a parallel extension of the mesh component.

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[7] Note that this is not contradictory with our finding of low overhead when comparing native and iMesh-based implementations, as the overhead measurements compare an iMesh implementation of a service to a non-iMesh implementation of that same functionality *for a given mesh database*.

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